Full wwPDB NMR Structure Validation Report (i)

Jun 12, 2024 – 02:35 PM EDT

PDB ID	:	1HJ7
Title	:	NMR study of a pair of LDL receptor Ca2+ binding epidermal growth factor-like domains, 20 structures
Authors	:	Saha, S.; Handford, P.A.; Campbell, I.D.; Downing, A.K.
Deposited on	:	2001-01-09

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

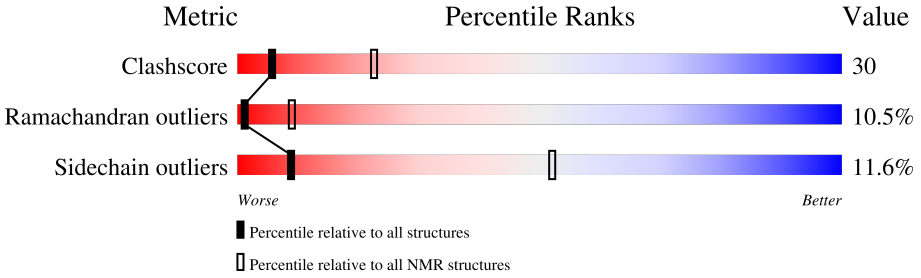
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	80	40% 51% 6% •

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:295-A:372 (78)	1.32	14

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 6, 8, 14, 15, 16, 18, 20
2	9, 12, 19
3	2, 3, 11
4	5, 10, 17
5	4, 7, 13

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1151 atoms, of which 542 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called LDL RECEPTOR.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	80	1149	361	542	105	129	12	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
			Total	Ca
2	A	2	2	2

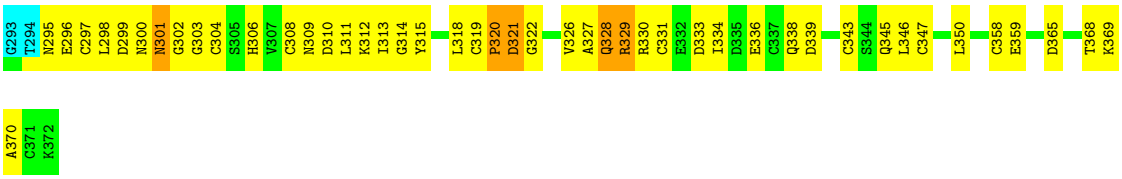
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: LDL RECEPTOR

Chain A: 40% 51% 6% •



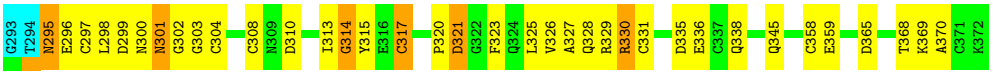
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: LDL RECEPTOR

Chain A: 52% 38% 8% •



4.2.2 Score per residue for model 2

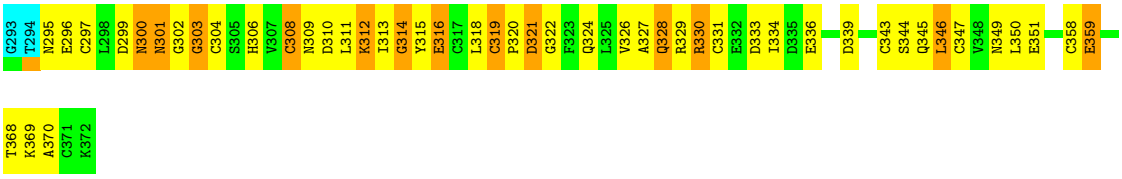
• Molecule 1: LDL RECEPTOR

Chain A: 46% 36% 15% •

4.2.3 Score per residue for model 3

- Molecule 1: LDL RECEPTOR

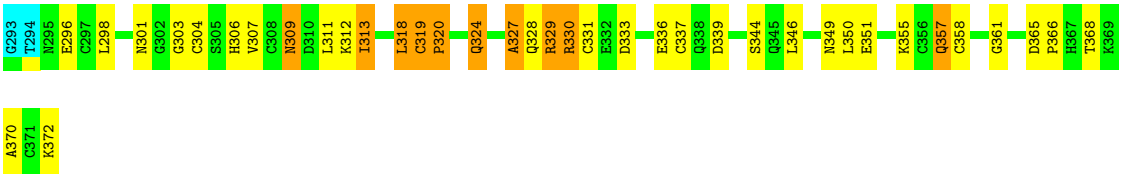
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: LDL RECEPTOR

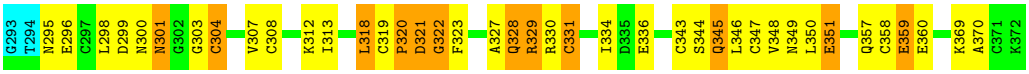
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: LDL RECEPTOR

Chain A:



4.2.6 Score per residue for model 6

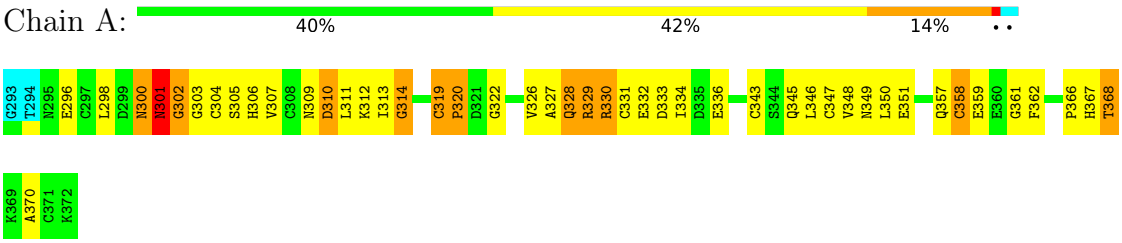
- Molecule 1: LDL RECEPTOR

Chain A:

4.2.7 Score per residue for model 7

- Molecule 1: LDL RECEPTOR

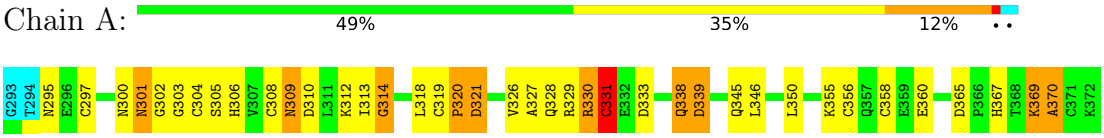
Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: LDL RECEPTOR

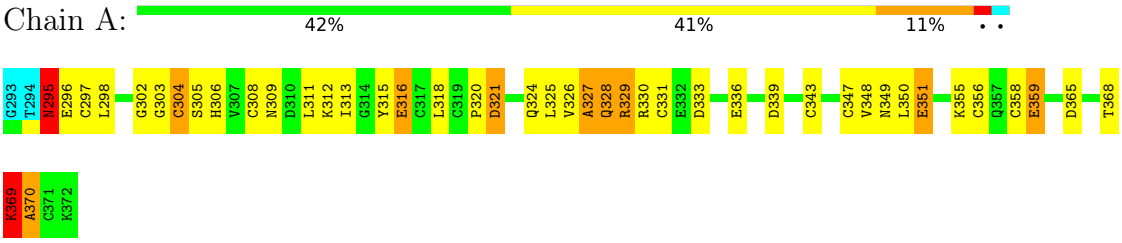
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: LDL RECEPTOR

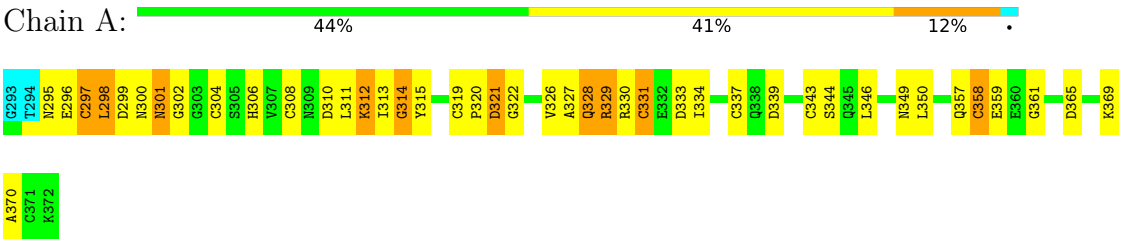
Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: LDL RECEPTOR

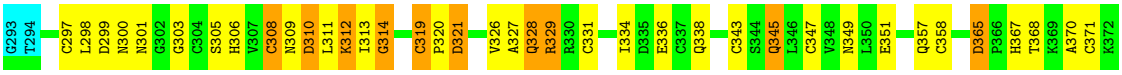
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: LDL RECEPTOR

Chain A: 50% 35% 12%



4.2.12 Score per residue for model 12

- Molecule 1: LDL RECEPTOR

Chain A: 45% 39% 11%

4.2.13 Score per residue for model 13

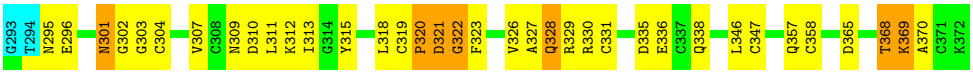
- Molecule 1: LDL RECEPTOR

Chain A: 60% 28% 10%

4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: LDL RECEPTOR

Chain A: 52% 36% 9%



4.2.15 Score per residue for model 15

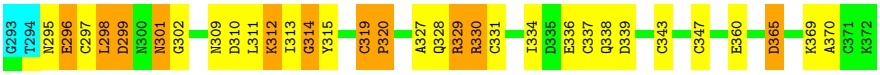
- Molecule 1: LDL RECEPTOR

Chain A: 41% 48% 8%

4.2.16 Score per residue for model 16

- Molecule 1: LDL RECEPTOR

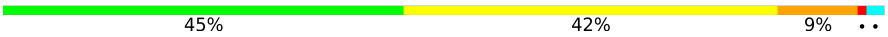
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: LDL RECEPTOR

Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: LDL RECEPTOR

Chain A:

4.2.19 Score per residue for model 19

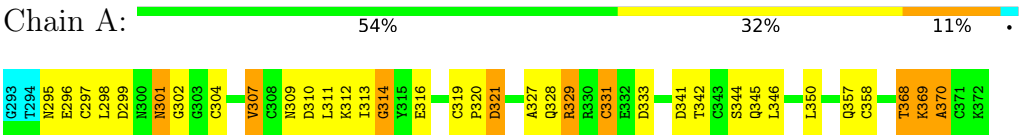
- Molecule 1: LDL RECEPTOR

Chain A:

4.2.20 Score per residue for model 20

- Molecule 1: LDL RECEPTOR

Chain A:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 280 calculated structures, 20 were deposited, based on the following criterion: *NO NOE, 3JHN OR 1JHN CONSTRAINTS VIOLATED BY > 0.5 A, 5 DEGREES OR 2 HERTZ*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	refinement	3.851
X-PLOR	structure solution	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	596	532	530	34±5
All	All	11960	10640	10600	686

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:320:PRO:O	1:A:322:GLY:N	0.87	2.07	19	4
1:A:326:VAL:HG13	1:A:327:ALA:H	0.76	1.40	17	3
1:A:298:LEU:HD22	1:A:298:LEU:N	0.67	2.04	20	6
1:A:297:CYS:O	1:A:299:ASP:N	0.67	2.27	16	2
1:A:343:CYS:SG	1:A:344:SER:N	0.66	2.68	3	4
1:A:326:VAL:HG13	1:A:327:ALA:N	0.65	2.06	11	3
1:A:368:THR:OG1	1:A:369:LYS:N	0.65	2.29	15	6
1:A:327:ALA:O	1:A:329:ARG:N	0.62	2.33	8	11
1:A:321:ASP:O	1:A:323:PHE:N	0.62	2.33	14	4
1:A:320:PRO:O	1:A:321:ASP:O	0.62	2.18	8	3
1:A:301:ASN:ND2	1:A:308:CYS:SG	0.60	2.74	19	2
1:A:311:LEU:O	1:A:313:ILE:N	0.60	2.34	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:306:HIS:ND1	1:A:319:CYS:SG	0.60	2.75	7	3
1:A:319:CYS:O	1:A:320:PRO:O	0.60	2.19	17	5
1:A:296:GLU:H	1:A:296:GLU:CD	0.59	2.01	7	1
1:A:345:GLN:NE2	1:A:356:CYS:SG	0.59	2.75	18	1
1:A:309:ASN:HD22	1:A:311:LEU:HD21	0.59	1.57	14	2
1:A:319:CYS:O	1:A:321:ASP:N	0.59	2.36	2	4
1:A:320:PRO:O	1:A:321:ASP:CB	0.58	2.52	1	8
1:A:336:GLU:N	1:A:349:ASN:HD21	0.58	1.96	19	2
1:A:300:ASN:O	1:A:302:GLY:N	0.57	2.38	7	1
1:A:327:ALA:O	1:A:328:GLN:CB	0.57	2.52	10	9
1:A:336:GLU:H	1:A:349:ASN:HD21	0.56	1.43	19	2
1:A:322:GLY:O	1:A:334:ILE:HG22	0.56	2.00	10	8
1:A:342:THR:CG2	1:A:354:TYR:CE2	0.56	2.88	15	1
1:A:295:ASN:HB2	1:A:298:LEU:HD22	0.56	1.78	5	1
1:A:306:HIS:CG	1:A:319:CYS:SG	0.56	2.98	6	3
1:A:298:LEU:N	1:A:298:LEU:CD2	0.56	2.68	11	6
1:A:320:PRO:O	1:A:321:ASP:C	0.56	2.45	18	6
1:A:369:LYS:CD	1:A:369:LYS:N	0.55	2.70	9	1
1:A:304:CYS:O	1:A:306:HIS:N	0.55	2.40	8	4
1:A:326:VAL:O	1:A:328:GLN:N	0.55	2.39	7	2
1:A:303:GLY:O	1:A:329:ARG:NH1	0.55	2.40	18	5
1:A:298:LEU:H	1:A:298:LEU:CD2	0.55	2.14	16	1
1:A:347:CYS:SG	1:A:347:CYS:O	0.55	2.64	3	5
1:A:304:CYS:SG	1:A:305:SER:N	0.55	2.80	9	1
1:A:365:ASP:OD1	1:A:369:LYS:N	0.55	2.39	10	1
1:A:298:LEU:N	1:A:298:LEU:CD1	0.54	2.70	5	1
1:A:348:VAL:CG1	1:A:350:LEU:HD21	0.54	2.32	7	1
1:A:297:CYS:O	1:A:301:ASN:N	0.54	2.40	16	2
1:A:301:ASN:ND2	1:A:304:CYS:O	0.54	2.41	8	7
1:A:301:ASN:ND2	1:A:304:CYS:N	0.54	2.55	17	1
1:A:296:GLU:N	1:A:296:GLU:OE1	0.54	2.40	6	9
1:A:345:GLN:HE22	1:A:364:LEU:HD21	0.54	1.63	18	1
1:A:299:ASP:O	1:A:301:ASN:N	0.54	2.41	6	5
1:A:336:GLU:OE1	1:A:349:ASN:ND2	0.54	2.41	7	3
1:A:302:GLY:O	1:A:304:CYS:N	0.54	2.41	8	6
1:A:301:ASN:O	1:A:301:ASN:ND2	0.54	2.41	3	4
1:A:329:ARG:HH11	1:A:329:ARG:CG	0.54	2.16	11	3
1:A:316:GLU:OE2	1:A:318:LEU:N	0.53	2.41	18	3
1:A:365:ASP:OD2	1:A:370:ALA:N	0.53	2.40	10	1
1:A:335:ASP:OD1	1:A:338:GLN:N	0.53	2.42	1	3
1:A:343:CYS:SG	1:A:346:LEU:O	0.53	2.67	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:344:SER:O	1:A:345:GLN:CB	0.53	2.55	18	3
1:A:346:LEU:N	1:A:346:LEU:HD22	0.53	2.18	14	4
1:A:329:ARG:CG	1:A:329:ARG:NH1	0.53	2.71	11	3
1:A:301:ASN:ND2	1:A:301:ASN:O	0.53	2.41	2	3
1:A:337:CYS:O	1:A:339:ASP:N	0.53	2.41	15	5
1:A:346:LEU:N	1:A:346:LEU:CD2	0.53	2.71	14	5
1:A:336:GLU:N	1:A:336:GLU:OE2	0.53	2.42	18	1
1:A:315:TYR:OH	1:A:329:ARG:NH1	0.53	2.42	12	2
1:A:330:ARG:NH1	1:A:330:ARG:CG	0.53	2.72	4	4
1:A:355:LYS:O	1:A:357:GLN:NE2	0.53	2.42	4	1
1:A:301:ASN:HD22	1:A:304:CYS:N	0.53	2.02	7	1
1:A:336:GLU:H	1:A:336:GLU:CD	0.52	2.08	13	15
1:A:365:ASP:OD2	1:A:367:HIS:NE2	0.52	2.42	8	1
1:A:368:THR:O	1:A:370:ALA:N	0.52	2.41	1	7
1:A:329:ARG:NH1	1:A:329:ARG:CG	0.52	2.72	20	3
1:A:338:GLN:N	1:A:338:GLN:OE1	0.52	2.41	17	1
1:A:330:ARG:O	1:A:331:CYS:SG	0.52	2.68	17	10
1:A:301:ASN:O	1:A:303:GLY:N	0.52	2.42	7	1
1:A:357:GLN:HE22	1:A:362:PHE:H	0.52	1.45	7	1
1:A:327:ALA:O	1:A:328:GLN:NE2	0.52	2.42	13	1
1:A:338:GLN:OE1	1:A:338:GLN:CA	0.52	2.57	17	1
1:A:341:ASP:OD1	1:A:342:THR:N	0.52	2.42	20	1
1:A:310:ASP:OD1	1:A:311:LEU:N	0.52	2.42	16	1
1:A:295:ASN:N	1:A:295:ASN:OD1	0.52	2.43	1	7
1:A:351:GLU:N	1:A:351:GLU:OE1	0.52	2.43	3	3
1:A:365:ASP:OD2	1:A:369:LYS:N	0.52	2.43	15	1
1:A:343:CYS:O	1:A:345:GLN:N	0.51	2.43	18	1
1:A:305:SER:O	1:A:306:HIS:CD2	0.51	2.63	9	2
1:A:351:GLU:H	1:A:351:GLU:CD	0.51	2.07	13	1
1:A:314:GLY:O	1:A:315:TYR:O	0.51	2.29	6	1
1:A:344:SER:O	1:A:345:GLN:CG	0.51	2.59	18	1
1:A:343:CYS:SG	1:A:357:GLN:N	0.51	2.83	10	2
1:A:337:CYS:H	1:A:349:ASN:HD22	0.51	1.47	19	1
1:A:360:GLU:H	1:A:360:GLU:CD	0.51	2.09	18	2
1:A:329:ARG:CG	1:A:329:ARG:HH11	0.51	2.18	2	3
1:A:297:CYS:SG	1:A:308:CYS:O	0.51	2.69	11	6
1:A:304:CYS:SG	1:A:329:ARG:O	0.51	2.69	5	1
1:A:357:GLN:O	1:A:358:CYS:SG	0.51	2.69	11	1
1:A:295:ASN:CB	1:A:298:LEU:HD22	0.51	2.36	5	1
1:A:300:ASN:O	1:A:301:ASN:CB	0.51	2.58	13	2
1:A:326:VAL:CG1	1:A:327:ALA:H	0.51	2.18	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:295:ASN:ND2	1:A:299:ASP:OD1	0.51	2.44	20	2
1:A:330:ARG:CG	1:A:330:ARG:HH11	0.51	2.18	7	3
1:A:326:VAL:O	1:A:327:ALA:HB3	0.51	2.06	2	1
1:A:327:ALA:O	1:A:328:GLN:CG	0.51	2.59	2	5
1:A:330:ARG:CG	1:A:331:CYS:H	0.51	2.19	9	3
1:A:368:THR:O	1:A:369:LYS:CB	0.51	2.59	13	1
1:A:315:TYR:HH	1:A:329:ARG:NH1	0.50	2.04	1	1
1:A:363:GLN:N	1:A:372:LYS:O	0.50	2.44	6	1
1:A:337:CYS:SG	1:A:337:CYS:O	0.50	2.70	16	1
1:A:371:CYS:SG	1:A:371:CYS:O	0.50	2.69	2	2
1:A:300:ASN:O	1:A:300:ASN:ND2	0.50	2.44	3	1
1:A:295:ASN:O	1:A:295:ASN:ND2	0.50	2.44	14	1
1:A:337:CYS:H	1:A:349:ASN:ND2	0.50	2.05	19	1
1:A:365:ASP:OD1	1:A:372:LYS:NZ	0.50	2.42	18	1
1:A:357:GLN:HE22	1:A:362:PHE:N	0.50	2.05	7	1
1:A:345:GLN:NE2	1:A:359:GLU:OE1	0.49	2.45	3	1
1:A:301:ASN:OD1	1:A:308:CYS:SG	0.49	2.70	6	1
1:A:324:GLN:NE2	1:A:333:ASP:O	0.49	2.45	6	2
1:A:304:CYS:SG	1:A:307:VAL:O	0.49	2.70	14	3
1:A:339:ASP:N	1:A:339:ASP:OD1	0.49	2.43	12	3
1:A:367:HIS:ND1	1:A:368:THR:N	0.49	2.61	18	2
1:A:326:VAL:O	1:A:326:VAL:HG22	0.49	2.08	12	2
1:A:326:VAL:CG1	1:A:330:ARG:O	0.49	2.61	6	1
1:A:365:ASP:OD2	1:A:367:HIS:CD2	0.49	2.66	8	1
1:A:296:GLU:N	1:A:296:GLU:OE2	0.49	2.45	12	1
1:A:345:GLN:NE2	1:A:371:CYS:SG	0.49	2.85	12	1
1:A:296:GLU:CB	1:A:315:TYR:CD2	0.49	2.95	19	1
1:A:302:GLY:C	1:A:304:CYS:H	0.49	2.11	1	6
1:A:365:ASP:OD2	1:A:372:LYS:NZ	0.49	2.42	4	1
1:A:318:LEU:O	1:A:319:CYS:SG	0.49	2.70	6	3
1:A:300:ASN:O	1:A:301:ASN:C	0.49	2.50	7	1
1:A:365:ASP:CG	1:A:369:LYS:N	0.49	2.66	15	2
1:A:360:GLU:N	1:A:360:GLU:OE2	0.49	2.45	16	1
1:A:326:VAL:CG1	1:A:327:ALA:N	0.49	2.75	11	4
1:A:295:ASN:N	1:A:310:ASP:OD2	0.49	2.46	3	1
1:A:363:GLN:N	1:A:363:GLN:OE1	0.49	2.46	19	1
1:A:359:GLU:O	1:A:361:GLY:N	0.49	2.45	18	1
1:A:364:LEU:HD13	1:A:365:ASP:N	0.48	2.22	18	2
1:A:307:VAL:HG12	1:A:308:CYS:N	0.48	2.23	15	2
1:A:313:ILE:O	1:A:314:GLY:O	0.48	2.31	11	10
1:A:307:VAL:CG1	1:A:308:CYS:N	0.48	2.76	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:297:CYS:O	1:A:298:LEU:C	0.48	2.51	16	2
1:A:295:ASN:O	1:A:297:CYS:N	0.48	2.46	16	1
1:A:355:LYS:O	1:A:356:CYS:SG	0.48	2.72	9	3
1:A:337:CYS:C	1:A:339:ASP:N	0.48	2.67	6	6
1:A:299:ASP:C	1:A:301:ASN:N	0.48	2.67	18	7
1:A:344:SER:O	1:A:358:CYS:SG	0.48	2.72	10	2
1:A:346:LEU:HD23	1:A:347:CYS:N	0.48	2.24	3	1
1:A:365:ASP:CB	1:A:368:THR:OG1	0.48	2.62	4	2
1:A:328:GLN:CG	1:A:328:GLN:O	0.48	2.61	3	2
1:A:296:GLU:CD	1:A:296:GLU:N	0.48	2.67	7	1
1:A:302:GLY:C	1:A:304:CYS:N	0.47	2.67	14	4
1:A:302:GLY:CA	1:A:315:TYR:OH	0.47	2.62	2	6
1:A:320:PRO:O	1:A:321:ASP:CG	0.47	2.53	11	4
1:A:359:GLU:CD	1:A:360:GLU:N	0.47	2.67	5	1
1:A:363:GLN:CD	1:A:364:LEU:N	0.47	2.68	18	1
1:A:297:CYS:SG	1:A:308:CYS:C	0.47	2.92	3	3
1:A:327:ALA:C	1:A:329:ARG:N	0.47	2.68	8	9
1:A:351:GLU:N	1:A:351:GLU:CD	0.47	2.67	3	1
1:A:368:THR:C	1:A:370:ALA:N	0.47	2.68	12	8
1:A:358:CYS:O	1:A:359:GLU:O	0.47	2.33	9	1
1:A:308:CYS:SG	1:A:308:CYS:O	0.47	2.72	13	1
1:A:304:CYS:C	1:A:306:HIS:N	0.47	2.67	8	4
1:A:363:GLN:N	1:A:363:GLN:CD	0.46	2.68	19	1
1:A:345:GLN:OE1	1:A:358:CYS:SG	0.46	2.73	1	2
1:A:330:ARG:CG	1:A:331:CYS:N	0.46	2.78	14	3
1:A:301:ASN:C	1:A:303:GLY:N	0.46	2.68	7	1
1:A:346:LEU:N	1:A:346:LEU:HD12	0.46	2.25	8	1
1:A:321:ASP:C	1:A:323:PHE:H	0.46	2.12	6	2
1:A:355:LYS:C	1:A:356:CYS:SG	0.46	2.94	9	2
1:A:317:CYS:O	1:A:325:LEU:HD13	0.46	2.10	18	2
1:A:330:ARG:CD	1:A:331:CYS:H	0.46	2.23	8	1
1:A:320:PRO:O	1:A:321:ASP:OD2	0.46	2.34	11	1
1:A:348:VAL:O	1:A:348:VAL:HG13	0.46	2.09	18	2
1:A:345:GLN:CG	1:A:356:CYS:SG	0.46	3.03	18	1
1:A:348:VAL:CG1	1:A:348:VAL:O	0.46	2.64	18	1
1:A:351:GLU:CD	1:A:351:GLU:N	0.46	2.67	13	1
1:A:318:LEU:C	1:A:319:CYS:SG	0.46	2.94	4	3
1:A:298:LEU:N	1:A:298:LEU:HD12	0.46	2.26	5	1
1:A:300:ASN:O	1:A:301:ASN:OD1	0.46	2.33	8	2
1:A:365:ASP:OD1	1:A:367:HIS:CD2	0.46	2.69	8	1
1:A:302:GLY:O	1:A:315:TYR:OH	0.46	2.34	12	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:364:LEU:HD11	1:A:369:LYS:O	0.46	2.10	13	1
1:A:335:ASP:CG	1:A:349:ASN:HD22	0.46	2.14	17	1
1:A:335:ASP:CG	1:A:349:ASN:ND2	0.46	2.69	17	1
1:A:320:PRO:C	1:A:322:GLY:N	0.46	2.68	19	1
1:A:326:VAL:HG23	1:A:327:ALA:N	0.46	2.25	19	1
1:A:357:GLN:C	1:A:358:CYS:SG	0.45	2.95	14	3
1:A:300:ASN:ND2	1:A:300:ASN:N	0.45	2.63	1	1
1:A:348:VAL:HG13	1:A:348:VAL:O	0.45	2.11	5	2
1:A:367:HIS:O	1:A:367:HIS:ND1	0.45	2.49	11	1
1:A:319:CYS:CB	1:A:320:PRO:CD	0.45	2.94	16	1
1:A:359:GLU:OE1	1:A:360:GLU:N	0.45	2.49	17	1
1:A:345:GLN:OE1	1:A:371:CYS:SG	0.45	2.74	18	1
1:A:344:SER:O	1:A:345:GLN:OE1	0.45	2.35	18	1
1:A:311:LEU:O	1:A:312:LYS:O	0.45	2.35	10	1
1:A:309:ASN:ND2	1:A:311:LEU:HD21	0.45	2.25	14	1
1:A:345:GLN:CD	1:A:356:CYS:SG	0.45	2.94	18	1
1:A:315:TYR:CD1	1:A:315:TYR:N	0.45	2.81	10	2
1:A:365:ASP:CG	1:A:370:ALA:N	0.45	2.69	10	1
1:A:297:CYS:SG	1:A:310:ASP:N	0.45	2.90	11	1
1:A:368:THR:O	1:A:369:LYS:CG	0.45	2.64	13	1
1:A:295:ASN:C	1:A:297:CYS:H	0.45	2.14	16	1
1:A:298:LEU:CD2	1:A:298:LEU:N	0.45	2.78	16	1
1:A:324:GLN:CG	1:A:325:LEU:N	0.45	2.80	9	1
1:A:296:GLU:OE1	1:A:310:ASP:OD1	0.45	2.34	16	2
1:A:296:GLU:OE1	1:A:310:ASP:OD2	0.44	2.35	6	6
1:A:299:ASP:C	1:A:301:ASN:H	0.44	2.16	2	5
1:A:367:HIS:N	1:A:367:HIS:ND1	0.44	2.56	2	1
1:A:298:LEU:N	1:A:298:LEU:HD22	0.44	2.26	16	1
1:A:296:GLU:OE2	1:A:310:ASP:OD2	0.44	2.34	19	1
1:A:338:GLN:OE1	1:A:338:GLN:O	0.44	2.36	1	3
1:A:365:ASP:N	1:A:370:ALA:O	0.44	2.49	8	1
1:A:319:CYS:SG	1:A:320:PRO:CD	0.44	3.05	11	1
1:A:345:GLN:CD	1:A:358:CYS:SG	0.44	2.95	11	1
1:A:343:CYS:SG	1:A:347:CYS:CB	0.44	3.05	16	1
1:A:311:LEU:O	1:A:312:LYS:C	0.44	2.56	17	9
1:A:327:ALA:C	1:A:329:ARG:H	0.44	2.15	4	3
1:A:359:GLU:CD	1:A:360:GLU:H	0.44	2.16	5	1
1:A:298:LEU:H	1:A:298:LEU:HD22	0.44	1.71	16	1
1:A:348:VAL:O	1:A:348:VAL:CG1	0.44	2.66	5	2
1:A:300:ASN:C	1:A:302:GLY:H	0.44	2.15	10	2
1:A:299:ASP:C	1:A:300:ASN:ND2	0.44	2.71	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:336:GLU:N	1:A:349:ASN:ND2	0.44	2.65	19	1
1:A:365:ASP:OD2	1:A:370:ALA:O	0.44	2.36	10	4
1:A:309:ASN:HD22	1:A:309:ASN:C	0.44	2.15	8	2
1:A:300:ASN:C	1:A:302:GLY:N	0.44	2.71	19	1
1:A:301:ASN:C	1:A:303:GLY:H	0.44	2.16	4	4
1:A:369:LYS:O	1:A:370:ALA:O	0.44	2.35	8	2
1:A:321:ASP:C	1:A:323:PHE:N	0.44	2.70	14	1
1:A:367:HIS:ND1	1:A:368:THR:OG1	0.44	2.44	7	1
1:A:333:ASP:OD2	1:A:350:LEU:O	0.43	2.36	9	12
1:A:334:ILE:O	1:A:336:GLU:OE2	0.43	2.36	11	6
1:A:325:LEU:HD11	1:A:328:GLN:HA	0.43	1.90	15	1
1:A:299:ASP:O	1:A:300:ASN:O	0.43	2.37	17	1
1:A:368:THR:C	1:A:370:ALA:H	0.43	2.15	12	5
1:A:324:GLN:OE1	1:A:333:ASP:O	0.43	2.37	4	1
1:A:327:ALA:O	1:A:328:GLN:C	0.43	2.56	9	4
1:A:365:ASP:OD1	1:A:370:ALA:O	0.43	2.37	11	5
1:A:345:GLN:OE1	1:A:359:GLU:OE1	0.43	2.36	3	1
1:A:307:VAL:O	1:A:318:LEU:N	0.43	2.51	4	1
1:A:333:ASP:OD2	1:A:349:ASN:OD1	0.43	2.36	10	2
1:A:330:ARG:O	1:A:331:CYS:O	0.43	2.36	6	2
1:A:306:HIS:CD2	1:A:306:HIS:N	0.43	2.87	4	1
1:A:363:GLN:NE2	1:A:364:LEU:N	0.43	2.67	18	1
1:A:336:GLU:OE1	1:A:349:ASN:OD1	0.43	2.36	3	4
1:A:333:ASP:OD2	1:A:351:GLU:OE2	0.43	2.37	7	1
1:A:365:ASP:CG	1:A:369:LYS:CA	0.43	2.87	15	1
1:A:300:ASN:O	1:A:301:ASN:CG	0.43	2.57	5	2
1:A:307:VAL:O	1:A:318:LEU:O	0.43	2.37	18	1
1:A:309:ASN:O	1:A:310:ASP:C	0.43	2.56	7	3
1:A:300:ASN:HD22	1:A:300:ASN:N	0.43	2.12	7	1
1:A:347:CYS:O	1:A:347:CYS:SG	0.43	2.77	11	2
1:A:326:VAL:O	1:A:327:ALA:C	0.43	2.56	9	1
1:A:302:GLY:O	1:A:329:ARG:NH2	0.43	2.51	10	2
1:A:297:CYS:C	1:A:299:ASP:N	0.42	2.72	16	2
1:A:350:LEU:O	1:A:351:GLU:O	0.42	2.36	5	1
1:A:335:ASP:CG	1:A:338:GLN:OE1	0.42	2.58	17	1
1:A:321:ASP:C	1:A:321:ASP:OD1	0.42	2.57	11	1
1:A:316:GLU:OE2	1:A:316:GLU:O	0.42	2.37	9	2
1:A:303:GLY:O	1:A:304:CYS:O	0.42	2.36	9	1
1:A:308:CYS:O	1:A:308:CYS:SG	0.42	2.77	15	2
1:A:345:GLN:HE22	1:A:359:GLU:CD	0.42	2.18	3	1
1:A:336:GLU:CD	1:A:336:GLU:N	0.42	2.73	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:296:GLU:N	1:A:296:GLU:CD	0.42	2.73	12	1
1:A:319:CYS:C	1:A:321:ASP:N	0.42	2.72	12	1
1:A:351:GLU:OE2	1:A:351:GLU:O	0.42	2.37	13	1
1:A:345:GLN:HE22	1:A:364:LEU:CD2	0.42	2.26	18	1
1:A:299:ASP:C	1:A:300:ASN:HD22	0.42	2.18	15	1
1:A:359:GLU:CD	1:A:359:GLU:N	0.42	2.73	1	1
1:A:337:CYS:C	1:A:339:ASP:H	0.42	2.18	10	1
1:A:306:HIS:NE2	1:A:330:ARG:NH2	0.42	2.68	18	1
1:A:297:CYS:C	1:A:298:LEU:HD22	0.42	2.34	20	1
1:A:364:LEU:HD13	1:A:364:LEU:C	0.42	2.34	2	1
1:A:337:CYS:O	1:A:337:CYS:SG	0.42	2.78	10	1
1:A:295:ASN:O	1:A:295:ASN:CG	0.42	2.57	17	2
1:A:303:GLY:CA	1:A:329:ARG:NH1	0.42	2.83	19	1
1:A:322:GLY:O	1:A:334:ILE:CG2	0.41	2.68	10	1
1:A:365:ASP:OD2	1:A:368:THR:OG1	0.41	2.37	19	2
1:A:330:ARG:O	1:A:331:CYS:CB	0.41	2.68	17	1
1:A:300:ASN:O	1:A:303:GLY:N	0.41	2.53	5	1
1:A:345:GLN:CG	1:A:346:LEU:N	0.41	2.83	18	1
1:A:325:LEU:HD12	1:A:331:CYS:SG	0.41	2.56	19	1
1:A:355:LYS:CB	1:A:355:LYS:NZ	0.41	2.84	17	1
1:A:328:GLN:O	1:A:328:GLN:CG	0.41	2.68	11	1
1:A:365:ASP:CG	1:A:370:ALA:H	0.41	2.19	10	1
1:A:326:VAL:CG2	1:A:327:ALA:N	0.41	2.83	19	1
1:A:302:GLY:CA	1:A:315:TYR:CZ	0.41	3.03	3	1
1:A:345:GLN:NE2	1:A:358:CYS:SG	0.41	2.94	7	1
1:A:367:HIS:ND1	1:A:367:HIS:N	0.41	2.68	12	1
1:A:296:GLU:OE1	1:A:296:GLU:CA	0.41	2.69	13	1
1:A:354:TYR:CD1	1:A:354:TYR:N	0.41	2.89	17	1
1:A:309:ASN:HD22	1:A:311:LEU:CD2	0.41	2.26	14	1
1:A:307:VAL:O	1:A:307:VAL:CG1	0.40	2.69	6	2
1:A:326:VAL:HG22	1:A:327:ALA:N	0.40	2.31	9	1
1:A:351:GLU:CA	1:A:351:GLU:OE1	0.40	2.69	9	1
1:A:358:CYS:O	1:A:359:GLU:C	0.40	2.60	12	1
1:A:356:CYS:O	1:A:357:GLN:CD	0.40	2.60	15	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	77/80 (96%)	51±3 (67±4%)	18±3 (23±4%)	8±2 (11±3%)	1 9
All	All	1540/1600 (96%)	1025 (67%)	353 (23%)	162 (11%)	1 9

All 32 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	328	GLN	20
1	A	321	ASP	15
1	A	369	LYS	13
1	A	320	PRO	12
1	A	312	LYS	11
1	A	314	GLY	10
1	A	313	ILE	9
1	A	303	GLY	5
1	A	361	GLY	5
1	A	331	CYS	5
1	A	345	GLN	5
1	A	370	ALA	5
1	A	295	ASN	5
1	A	300	ASN	5
1	A	326	VAL	4
1	A	327	ALA	4
1	A	366	PRO	4
1	A	322	GLY	3
1	A	359	GLU	3
1	A	315	TYR	2
1	A	310	ASP	2
1	A	360	GLU	2
1	A	298	LEU	2
1	A	338	GLN	2
1	A	344	SER	2
1	A	351	GLU	1
1	A	301	ASN	1
1	A	302	GLY	1
1	A	305	SER	1
1	A	304	CYS	1
1	A	296	GLU	1
1	A	299	ASP	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	69/70 (99%)	61±2 (88±4%)	8±2 (12±4%)	9 52
All	All	1380/1400 (99%)	1220 (88%)	160 (12%)	9 52

All 44 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	301	ASN	13
1	A	329	ARG	13
1	A	331	CYS	10
1	A	358	CYS	10
1	A	319	CYS	9
1	A	309	ASN	8
1	A	330	ARG	7
1	A	343	CYS	6
1	A	295	ASN	5
1	A	297	CYS	5
1	A	368	THR	5
1	A	339	ASP	5
1	A	324	GLN	4
1	A	308	CYS	4
1	A	316	GLU	4
1	A	367	HIS	3
1	A	359	GLU	3
1	A	304	CYS	3
1	A	347	CYS	3
1	A	338	GLN	3
1	A	351	GLU	3
1	A	317	CYS	2
1	A	346	LEU	2
1	A	364	LEU	2
1	A	300	ASN	2
1	A	318	LEU	2
1	A	310	ASP	2
1	A	356	CYS	2
1	A	369	LYS	2

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Mol	Chain	Res	Type	Models (Total)
1	A	299	ASP	2
1	A	365	ASP	2
1	A	321	ASP	2
1	A	344	SER	1
1	A	357	GLN	1
1	A	305	SER	1
1	A	332	GLU	1
1	A	312	LYS	1
1	A	371	CYS	1
1	A	328	GLN	1
1	A	296	GLU	1
1	A	345	GLN	1
1	A	372	LYS	1
1	A	355	LYS	1
1	A	307	VAL	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided